Critical manifold of the Potts model: Exact results and homogeneity approximation

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Abstract

The q-state Potts model has stood at the frontier of research in statistical mechanics for many years. In the absence of a closed-form solution, much of the past efforts have focused on locating its critical manifold, trajectory in the parameter $\{q, e^J\}$ space where J is the reduced interaction, along which the free energy is singular. However, except in isolated cases, antiferromagnetic (AF) models with $J < 0$ have been largely neglected. In this paper we consider the Potts model with AF interactions focusing on obtaining its critical manifold in exact and/or closed-form expressions.

We first re-examine the known critical frontiers in light of AF interactions. For the square lattice we confirm the Potts self-dual point to be the sole critical frontier for $J > 0$. We also locate its critical frontier for $J < 0$ and find it to coincide with a solvability condition observed by Baxter in 1982. For the honeycomb lattice we show that the known critical frontier holds for all J, and determine its critical $q_c = \frac{1}{2}(3 + \sqrt{5}) = 2.61803$ beyond which there is no transition. For the triangular lattice we confirm the known critical frontier to hold only for $J > 0$.

More generally we consider the centered-triangle (CT) and Union-Jack (UJ) lattices consisting of mixed J and K interactions, and deduce critical manifolds under homogeneity hypotheses. For $K = 0$ the CT lattice is the diced lattice, and we determine its critical manifold for all J and find $q_c = 3.32472$. For $K = 0$ the UJ lattice is the square lattice and from this we deduce both the $J > 0$ and $J < 0$ critical manifolds and $q_c = 3$. Our theoretical predictions are compared with recent numerical results.

PACS numbers: 05.50.+q, 02.50.-r, 64.60.Cn

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The Potts model, proposed by Potts exactly sixty years ago [1], has been at the forefront of interest throughout the years. The Potts model extends the 2-state Ising model to $q > 2$ states (for reviews on relevances of the Potts model see [2, 3]). Despite the intense interest, however, the general q-state Potts model has remained unsolved. An equivalent and more revealing formulation of the Potts model is the random cluster model advanced by Kasteleyn and Fortuin [4, 5]. In this formulation the partition function is written as a sum of randomly connected cluster of lattice sites with edge weights $v = e^J - 1$, where J is the Potts interaction with $J > 0$ (resp. < 0) indicating ferromagnetic (resp. antiferromagnetic (AF)) interactions. The number of spin states q then emerges as a cluster weighting factor, thus providing a powerful means of continuing the Potts model to non-integral values of q. In the limit of $q \to 1$, for example, the formulation leads to a bond percolation with edge occupation probability $p = 1 - e^{-J}$.

Most studies of the Potts model have focused on ferromagnetic interactions, and the AF models have been largely neglected. (See however [6, 7] where the AF Potts model is discussed in the context of field theory.) For $J < 0$, the cluster weights which are products of edge weights v, can be either positive or negative resulting in a delicate cancelation. Since most analyses are based on a positivity assumption of Boltzmann weights, they are not applicable to AF models. In the percolation limit, for example, the edge occupying probability becomes negative losing its physical meaning.

In the absence of closed-form solutions, efforts have focused on determining its critical manifold, or critical frontier, a trajectory in the $\{q, e^J\}$ parameter space along which the free energy becomes singular. But known critical manifold of the Potts model are very few. They are limited to the square, honeycomb and triangular lattices given by

$$v^2 = q \quad \text{(square)} \tag{1}$$

$$v^3 - 3qv - q^2 = 0 \quad \text{(honeycomb)} \tag{2}$$

$$v^3 + 3v^2 - q = 0. \quad \text{(triangular)} \tag{3}$$

Here, we examine closely the applicability of (1) - (3) to AF interactions.

The critical point (1) for the square lattice was obtained by Potts [1] using the duality relation [2]

$$(e^J - 1)(e^{J^*} - 1) = q \tag{4}$$

relating an interaction J to a J^* on the dual lattice. Since the square lattice is self-dual

and assuming a unique transition, the duality (4) determines the critical point at $J = J^*$ or $v^2 = q$. This works only for $J > 0$. For $J < 0$ and $q > 1$, (4) relates J to a dual J^* in the complex-temperature plane. The self-dual argument fails and (1) does not hold.

In 1982, Baxter [8] observed that the AF Potts model on the square lattice is exactly solvable at

$$(e^J + 1)^2 = 4 - q, \qquad (q \leq 3) \tag{5}$$

and argued that the condition (5) should coincide with the critical point as in the case of the ferromagnetic model. Indeed, as we shall see below, the condition (5) emerges as the AF branch of the Potts critical manifold when the square lattice is considered in the larger setting of a Union-Jack lattice.

One important feature of the $J < 0$ transition is the existence of a critical q_c beyond which there is no transition. The disappearance of a transition for large q in any AF model is expected on general ground since for q sufficiently large the ground state entropy will destroy any transition. But the actual determination of q_c is lattice-dependent. For the square lattice, for example, (5) gives $q_c = 3$.

The critical points (2) and (3) for the honeycomb and triangular lattices can be derived as follows: Consider a triangular Potts lattice whose Hamiltonian is separable into sum over individual up-pointing triangles so that the partition function can be written as

$$Z = \sum_{s_i=1}^{q} \prod_{\triangle} W(s_1, s_2, s_3), \tag{6}$$

where $W(s_1, s_2, s_3)$ is the Boltzmann weight of an individual triangle with 3 corner spins s_1, s_2, s_3; the product is taken over all up-pointing triangles. An example is the honeycomb lattice divided into triangles shown in Fig.1(a). Clearly, properties of this Potts model are completely determined by the weights $W(s_1, s_2, s_3)$.

Baxter *et al* [9] (see also Wu and Lin [10]) have obtained a self-dual trajectory for a triangular Potts model with 2- and 3-site interactions. In terms of the W-weights the self-dual trajectory can be recast as

$$W(1,1,1) = 3\,W(1,1,2) + (q-2)\,W(1,2,3). \tag{7}$$

Wu and Zia [11] have further established that, for positive $W(s_1, s_2, s_3)$ and in the regime $W(1,1,1)$ dominates, or

$$W(1,1,1) > \{W(1,1,2),\, W(1,2,3)\} > 0, \tag{8}$$

there is a transition into a ferromagnetic ordered state on the underlying triangular lattice at the self-dual point (7). Indeed, for $W > 0$ the self-dual trajectory (7) lies entirely in the regime (8). The transition is expected to be continuous for $q \le 4$ and of first order for $q > 4$ from universality considerations [2]. In the regime where $W(1,2,3)$ dominates and for $q = 3$, there exists a transition into an antiferromagnetic ordered state which has a 6-fold degenerate ground state. But the critical manifold for this transition in terms of the W-weights is not known.

We now specialize (7) to specific lattices. For the honeycomb Potts lattice we take as the individual up-pointing triangles the setup in Fig. 1(a). This gives after tracing over the center spin s_0,

$$W(1,1,1) = e^{3J} + q - 1,\ W(1,1,2) = e^{2J} + e^{J} + q - 2,\ W(1,2,3) = 3e^{J} + q - 3. \qquad (9)$$

Substituting (9) into (7) we obtain the critical point (2). Since $W \ge 0$ for all (positive and negative) J, the critical manifold (2) holds for *all* J and gives the critical q_c as the root of

$$q^2 - 3q + 1 = 0, \qquad \text{(honeycomb)} \qquad (10)$$

or $q_c = \frac{1}{2}(3 + \sqrt{5}) = 2.61803....$

For latter use we recast the critical manifold (7) in another language. The star-triangle transformation of Fig. 1 transforms the honeycomb lattice to a triangular lattice with 2-site interactions K' and 3-site interactions M in every up-pointing triangle. A little algebra shows that the critical manifold (7) can be written as

$$e^{3K'+M} - 3\ e^{K'} - (q-2) = 0, \qquad (11)$$

with

$$e^{3K'+M} = \frac{e^{3J} + q - 1}{3e^{J} + q - 3}, \quad e^{K'} = \frac{e^{2J} + e^{J} + q - 2}{3e^{J} + q - 3}. \qquad (12)$$

Now turning to the triangular Potts lattice for which each individual triangle consists of 3 edges of interactions J, we have

$$W(1,1,1) = e^{3J}, \qquad W(1,1,2) = e^{J}, \qquad W(1,2,3) = 1. \qquad (13)$$

For $J > 0$ the weights (13) are in the regime (8) and the substitution of (13) into (7) leads to the critical manifold (3). For $J < 0$ and $q = 3$, the weights (13) are in the AF regime.

The location of its critical point has been the subject matter of several studies. From low-temperature series of the partition function Enting and Wu [12] determined a first-order transition at the critical point $e^{J_c} = 0.204$. Adler *et al* [13] found $e^{J_c} = 0.20309 \pm 0.00003$ from Monte Carlo simulations, and Chang et al [14] found $e^{J_c} = 0.203073(20)$ from transfer-matrix computations. Feldmann *et al* [15] showed this transition to be consistent with a complex singularity in the dual honeycomb lattice [16].

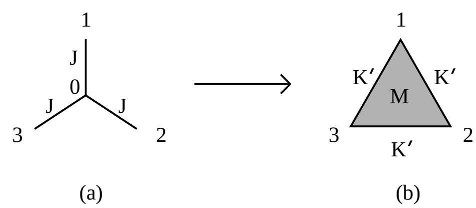

FIG. 1. A star-triangle transformation. The 'star' in (a) is mapped into a triangle in (b) consisting of 2-spin interactions K' and 3-spin interaction M.

We consider next the critical point of the diced lattice, a subject matter of recent studies [17, 18]. The diced lattice is the lattice in Fig. 2(a) with the heavy edges K removed. In 1979, one of us [19] (see also [20]) introduced a homogeneity hypothesis and derived a conjectured critical manifold for the diced lattice. The derivation of the homogeneity hypothesis is as follows:

Apply the star-triangle transformation of Fig. 1 to all 3-coordinated sites of the diced lattice. This results in a triangular lattice with 2-site interactions $2K'$ and 3-site interactions M in *every* face with $e^{K'}$ and e^M given by (12). If the interaction M exists in only the up-pointing triangular faces, the exact critical frontier is (11) with $K' \to 2K'$. The idea of homogeneity hypothesis, which we shall later extend to the Union-Jack lattice, is to postulate that when 3-site interactions M and M' are present in alternating faces, the critical frontier is (11) modified by replacing $M \to M + M'$ in the exponential. In the case of diced lattice where $M' = M$, this gives the critical manifold (11) with $K' \to 2K', M \to 2M$. This is the homogeneity approximation (HA).

The resulting critical manifold can be written in a generic form

$$W^2(1,1,1) = 3\,W^2(1,1,2) + (q-2)\;W^2(1,2,3) \qquad \text{(HA)} \qquad (14)$$

with W-weights given in (9). Explicitly, (14) reads

$$v^6 + 6v^5 + 12v^4 + 2qv^3 - 9qv^2 - 6q^2v - q^3 = 0. \qquad \text{(HA – diced lattice)} \tag{15}$$

The critical manifold for the kagome lattice is the dual of (15), or

$$v^6 + 6v^5 + 9v^4 - 2qv^3 - 12qv^2 - 6q^2v - q^3 = 0. \qquad \text{(HA – kagome lattice)} \tag{16}$$

This is the conjecture advanced in [19]. In the case of $M \neq M'$ and the up- and down-pointing triangular faces have different weights $W_\triangle$ and $W_\bigtriangledown$, the generalization of (14) is to replace W^2 by $W_\triangle \cdot W_\bigtriangledown$.

The critical manifolds (15) and (16) are exact for the Ising model $q = 2$. At $q = 2$ (15) gives the solution $\cosh J = (\sqrt{3}+1)/2$ and (16) has only one solution at $e^J = \sqrt{3+2\sqrt{3}} = 2.5424598$. both in agreement with Syozi [21].

At $q = 3$, (15) has six roots, $(e^J)_{\rm diced} = v+1 = 2.598917, 0.121599, -2.255914, -0.462026$, and $-0.00128784 \pm 1.742380\ i$. The first 2 roots give respective $J > 0$ and $J < 0$ critical points. The other 4 solutions are outside the regime (8) and are not singular points, so they are discarded. The $J > 0$ transition point $e^J = 2.598917$ is within 0.002% of the high-precision value $e^J = 2.598755(6)$ from a preliminary finite-size analysis [22]. But the $J < 0$ transition point 0.121599 differs by about 8% from the value 0.1393650(4) from the same finite-size analysis. Earlier numerical estimates include 0.1394 and 0.1380 of Kotecky *et al* [17] and Chen *et al* [18], and the value 0.1393(8) of Feldmann *et al* [23] computed from a complex-temperature singularity of the dual kagome lattice [16]. All these values are consistent with the precise determination 0.139365 of [22]. The relatively sizable discrepancy of the HA prediction indicates its inadequacy for AF interactions.

At $v = -1$ (15) determines q_c for the diced lattice from

$$q^3 - 6q^2 + 11q - 7 = 0, \qquad \text{(diced)} \tag{17}$$

or $q_c = 3.32472$. This is compared to the bound $q_c = 3.117689$ argued by Kotecky *et al* [17] and the more precise value $q_c = 3.4380(2)$ from finite-size analysis [22].

The critical points of the kagome lattice are the dual of those of the diced lattice. For $q = 3$ the singularity at 2.598917 of the diced gives a corresponding kagome critical point 2.876269 which has been shown [24] to be of the same high accuracy as the diced solution. The dual of the AF singularity is complex having no physical meaning. So there is only

a single (ferromagnetic) transition in the kagome lattice. Note that a direct evaluation of (16) yields a spurious AF solution $e^{J_c} = 0.078600$ which is the dual of the discarded diced solution -2.255914 not representing a singularity.

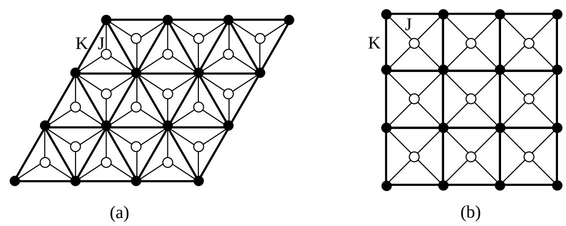

FIG. 2. (a) The centered-triangle lattice constructed by inserting sites (open circles) to faces of the triangular lattice. (b) The Union-Jack lattice.

We consider next the centered-triangular (CT) and Union-Jack (UJ) lattices shown in Fig. 2. The CT lattice, also known as the asanoha or hemp-leaf lattice [21], is a triangular lattice with a spin inserted in each triangular face. Similarly the UJ lattice can be regarded as a centered-square lattice. These lattices have received considerable recent attention as instances of finite-temperature transitions in AF Potts models [17, 18, 25].

For the CT lattice we trace over all 3-coordinated sites. This leads to a triangular lattice with 2-site interactions $K+2K'$ and 3-site interactions M in every face. Then, as in the case of the diced lattice, the homogeneity CT critical manifold is (11) with $K' \to K+2K', M \to 2M$. This leads to the critical manifold (14) with

$$\begin{aligned} W(1,1,1) &= e^{3K/2}(e^{3J}+q-1), \\ W(1,1,2) &= e^{K/2}(e^{2J}+e^{J}+q-2), \\ W(1,2,3) &= 3e^{J}+q-3. \end{aligned} \tag{18}$$

(Note the split of the interaction K into two parallel $K/2$.) Explicitly, the critical manifold reads

$$e^{3K}(e^{3J}+q-1)^2 = 3\,e^{K}(e^{2J}+e^{J}+q-2)^2+(q-2)(3e^{J}+q-3)^2, \quad (\mathrm{HA-CT\ lattice}) \tag{19}$$

which is to hold in regime (8) with W-weights (18).

The critical manifold (19) is exact for the Ising model since the star-triangle transformation is exact for $q=2$. This gives $2\cosh J = 1+\sqrt{3}\,e^{-K}$. In the general case we have considered the solution of (19) for $|K|=|J|$. We find $q=3$ solutions $e^{J}=e^{K}=1.596063$

and $e^J = e^{-K} = 0.602542$. These values are accurate to within 5 decimal places when compared with results of a preliminary finite-size analysis [22]. There is no $K < 0, |J| = |K|$ solution.

The Union-Jack is the lattice shown in Fig. 2(b). In order to extend the homogeneity consideration, we consider first the anisotropic UJ lattice with a unit cell shown in Fig. 3(a). Setting $J_4 = 0$ as in Fig. 3(b), the UJ lattice becomes the triangular lattice in Fig. 4 with J_1, J_2, J_3 interactions in up-pointing triangular faces. The critical manifold of this triangular lattice is the anisotropic version of (7) [11], namely.

$$W(1,1,1) = W(1,2,2) + W(2,1,2) + W(2,2,1) \ + (q-2)\ W(1,2,3). \tag{20}$$

Here (20) is to hold in the regime $W > 0$ and $W(1,1,1)$ dominates, and the transition is to a state of ferromagnetic ordering.

The W-weights in (20) can be read off from Fig. 3(b),

$$\begin{aligned}
W(1,1,1) &= e^{K_1+K_2}(e^{J_1+J_2+J_3} + q - 1), \\
W(1,2,2) &= e^{K_2}(e^{J_1} + e^{J_2+J_3} + q - 2), \\
W(2,1,2) &= e^{J_2} + e^{J_1+J_3} + q - 2, \\
W(2,2,1) &= e^{K_1}(e^{J_3} + e^{J_1+J_2} + q - 2), \\
W(1,2,3) &= e^{J_1} + e^{J_2} + e^{J_3} + q - 3,
\end{aligned} \tag{21}$$

and the critical manifold (20) with (21) is exact.

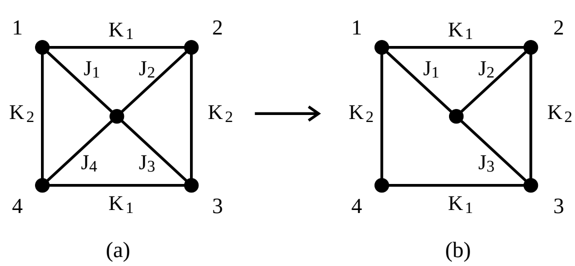

FIG. 3. (a) Union-Jack lattice with anisotropic interactions. (b) The $J_4 = 0$ Union-Jack lattice.

Now consider the Union-Jack lattice with $J_4 \neq 0$. As in the case of the CT lattice, we introduce the homogeneity hypothesis by inserting J_4 into (20) such that the resulting expression retains appropriate symmetries of the 4 interactions J_1, J_2, J_3, J_4, and reduces to (20) when J_4 is set to zero. The simplest way to do this is to insert J_4 into appropriate

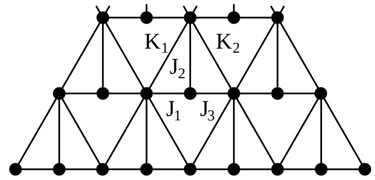

FIG. 4. A triangular lattice with J interactions in every up-pointing triangular face.

exponents in $W(1,1,1), W(1,2,2), W(2,1,2), W(2,2,1)$ and insert $e^{J_4}-1$ into $W(1,2,3)$. This gives rise to the following homogeneity approximation for the anisotropic UJ lattice,

$$\begin{aligned} e^{K_1+K_2}(e^{J_1+J_2+J_3+J_4}+q-1) = e^{K_2}(e^{J_1+J_4}+e^{J_2+J_3}+q-2) \\ + e^{K_1}(e^{J_3+J_4}+e^{J_1+J_2}+q-2) + e^{J_2+J_4}+e^{J_1+J_3}+q-2 \\ + (q-2)(e^{J_1}+e^{J_2}+e^{J_3}+e^{J_4}+q-4). \end{aligned} \tag{22}$$

When $K_1 = K_2 = 0$, (22) reduces to the critical manifold of the checkerboard lattice conjectured in [19]. However, when $K_1 \neq K_2$ the expression (22) lacks the intrinsic symmetry of $J_1 \leftrightarrow J_3$ or $J_2 \leftrightarrow J_4$. For the isotropic lattice $J_1 = J_2 = J_3 = J_4 = J$ we are interested in, we obtain

$$e^{K_1+K_2}(e^{4J}+q-1) = (e^{K_1}+e^{K_2})(2e^{2J}+q-2) + 2\ e^{2J} + 4(q-2)e^{J} + (q-2)(q-3). \qquad (\mathrm{HA-Union\ Jack\ lattice}) \tag{23}$$

This is the homogeneity approximation for the Union-Jack lattice.

The manifolds (22) and (23) are exact at $q = 2$ as they reproduce the known Ising critical point obtained by Wu and Lin [26]. When $J = 0$, the Union-Jack lattice reduces to a square lattice with anisotropic interactions K_1 and K_2, and (23) gives the known critical point $(e^{K_1}-1)(e^{K_2}-1) = q$. When $K_1 = K_2 = 0$, the Union-Jack lattice reduces to a square lattice of interactions J and (23) factorizes into

$$[(e^J-1)^2-q]\ [e^{2J}+2e^J+q-3] = 0. \tag{24}$$

Setting the first factor equal to zero gives the critical frontier (1). Setting the second factor equal to zero gives the Baxter solvability condition (5) as the $J < 0$ critical frontier as alluded to earlier.

In the general case we have considered the solution of (23) for $|K| = |J|$. For $q = 3$ we found solutions $e^J = e^K = 1.80168$ and $e^J = e^{-K} = 0.49256$. In addition, there is an AF

solution in $2 \le q \le 3$ at, for example, $e^K = e^J = 0.081504$ at $q = 2.5$. This solution is an extension of the $J < 0$ transition (5). For $K_1 = K_2 = K$ and setting $e^K = e^J = 0$ in (23), we obtain $q_c = 3$. Indeed, numerically we found no $K = J < 0$ solution of (23) in $q > 3$. We remark that Chen *et al* [18] have recently studied the $q = 4$, $K = J < 0$, Union-Jack model (see also [25]) using a tensor-based numerical method, and found an 'entropy-driven' transition at $e^K = e^J = 0.0523$. Since we found $q_c = 3$ for transitions to ferromagnetic ordering on the underlying square lattice, the transition at $q = 4$ is likely of a different nature as described and argued by Deng et al [25].

Finally we remark that since the duals of the CT and UJ lattices are, respectively, the 3-12 and 4-8, or $(3,\ 12^2)$ and $(4,\ 8^2)$, lattices, the duals of (19) and (23) give the critical manifolds for the 3-12 and 4-8 lattices. In the case of uniform interactions $K = K_1 = K_2 = J$, we obtain

$$\begin{aligned} v^7(v+3)^2 &= q[3v^7 + (q+32)v^6 + 15(2q+5)v^5 + q(12q+111)v^4 + 2q^2(q+41)v^3 \\ &\quad + 36q^3v^2 + 9q^4v + q^5], \qquad (3-12\ \text{lattice}) \qquad (25) \\ v^6 + 4v^5 &= q\ (v^4 + 16v^3 + 15qv^2 + 6q^2v + q^3), \qquad (4-8\ \text{lattice}) \qquad (26) \end{aligned}$$

where $v = e^J - 1$. Both (25) and (26) are exact at $q = 2$ reproducing the known Ising critical points [21], and have only ferromagnetic solutions. At $q = 1$ (25) and (26) give the bond percolation thresholds $(p_c)_{3-12} = 0.740423$ and $(p_c)_{4-8} = 0.676835$ in agreement with prior numerical estimations [29].

In summary, we have considered a lingering unsettled question on critical manifolds of Potts models with AF interactions. We have re-examined the known critical frontiers of the square, honeycomb and the triangular lattices in light of AF interactions. We have also examined the critical manifolds of the diced and kagome lattices under a homogeneity assumption, and extended the homogeneity consideration to centered-triangular and Union-Jack lattices to deduce critical manifolds. Our theoretical predictions are compared with results of several recent numerical studies.

After the completion of this work, we received a preprint [27] on a new graphical analysis of the Potts critical manifold which identifies the kagome conjecture (16) as a first-order approximant, thus resolving the long-standing question on the exactness of the conjecture. In [27] the AF critical line (5) is also deduced from the checkerboard manifold. We thank J. L. Jacobsen for sending a copy of [27] prior to publication. The identification of the

homogeneity approximation as a first-order approximant in the graphical analysis can also be extended to (23) for $K_1 = K_2$ [28]. We would like to thank R. Shrock for comments and suggestions and calling attention to [14–16], and thank J. Salas and R. Ziff for comments. We thank Z. Fu for help in the preparation of the manuscript. The work of WG is supported by the National Science Foundation of China (NSFC) under Grant No. 11175018, and by the program for New Century Excellent Talents in University (NCET-08-0053).

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